

Supporting Information

Imidazopyridine/Pyrrole and Hydroxybenzimidazole/Pyrrole Pairs for DNA Minor Groove Recognition

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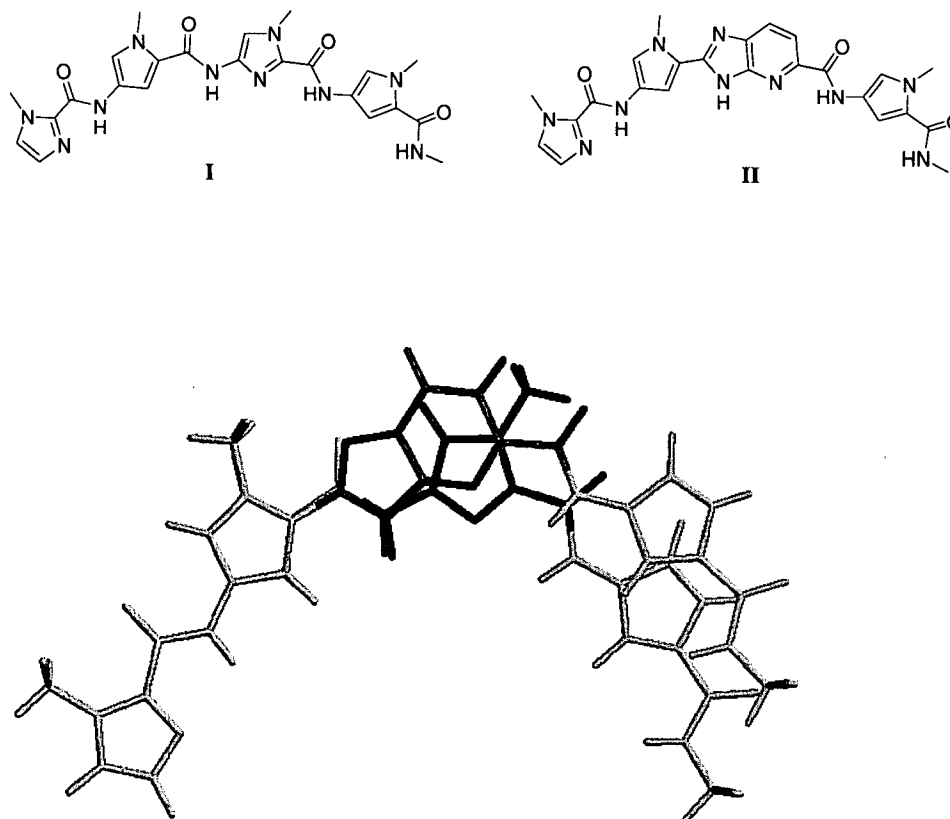


Figure S1. Minimized overlaid geometries of four-ring polyamide subunits MeNHCOPyImPyIm (I) and MeNHCOPyIpPyIm (II).^[a]

^[a] Gas-phase ab initio HF/6-31G* energy minimization; Spartan Essential Software, Wavefunction Inc., 2001.

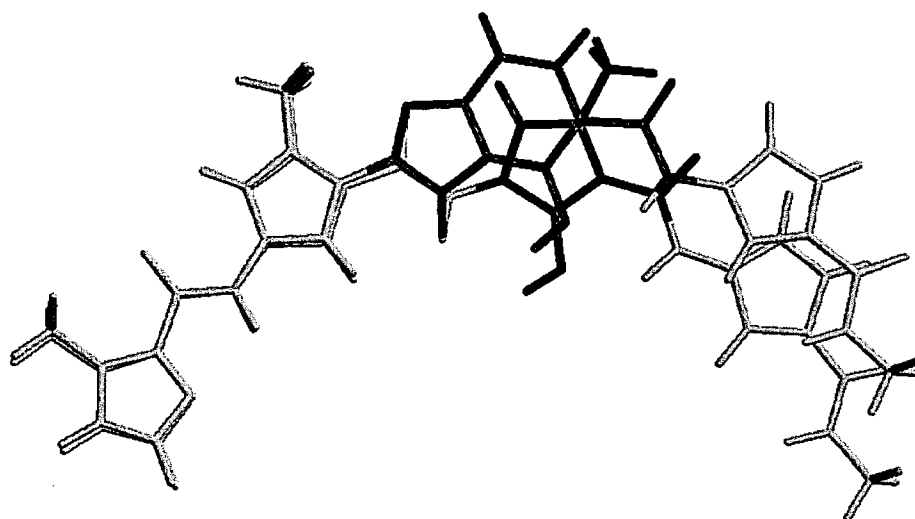
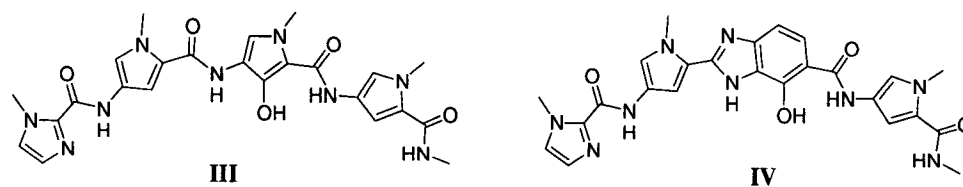


Figure S2. Minimized overlaid geometries of four-ring polyamide subunits MeNHCOPyHpPyIm (III) and MeNHCOPyHzPyIm (IV).^[a]

^[a] Gas-phase ab initio HF/6-31G* energy minimization; Spartan Essential Software, Wavefunction Inc., 2001.

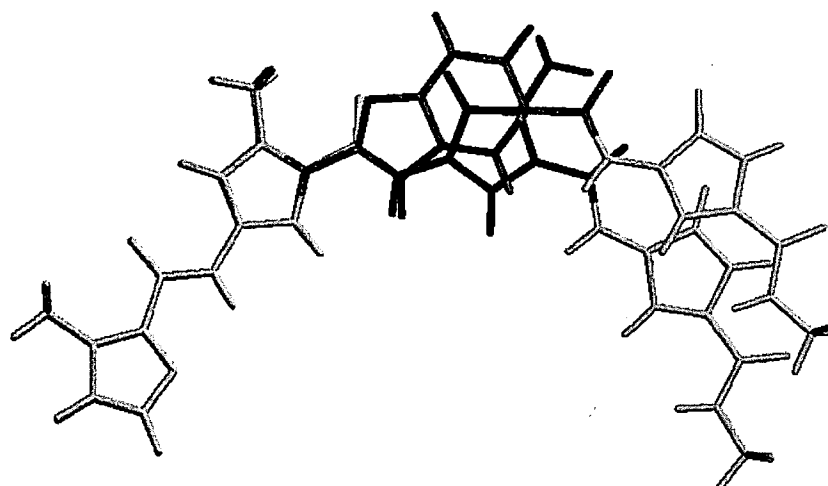
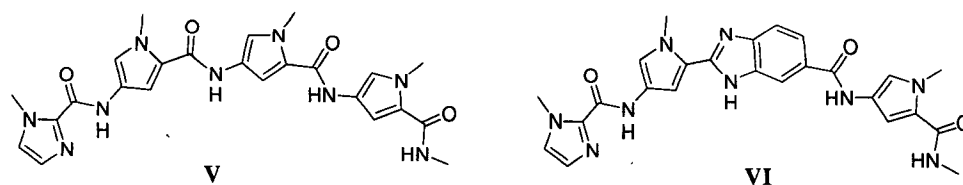


Figure S3. Minimized overlaid geometries of four-ring polyamide subunits MeNHCOPyPyPyIm (V) and MeNHCOPyBiPyIm (VI).^[a]

^[a] Gas-phase ab initio HF/6-31G* energy minimization; Spartan Essential Software, Wavefunction Inc., 2001.